

Diisopropyl fluorophosphate
55-91-4 | DTXSID1040667

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.28

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 7.00e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diisopropyl fluorophosphate</div> <div>Measured: 1.17</div> <div>Predicted: 1.28</div>	<div>Image not found</div> <div>Tripropyl phosphate</div> <div>Measured: 1.87</div> <div>Predicted: 1.92</div>	<div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: 0.8</div> <div>Predicted: 8.20e-01</div>
<div>Image not found</div> <div>Tripropyl phosphite</div> <div>Measured: 2.26</div> <div>Predicted: 2.32</div>	<div>Image not found</div> <div>1-hexyl-5-oxopyrrolidine-3-carboxylic acid</div> <div>Measured: 1.60</div> <div>Predicted: 1.80</div>	